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ME469: A Verification and Validation (V&V) Methodology (Review)

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SAND2018-4536 PE

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Verification vs Validation (V&V)? The Formal Lexicon (REVIEW)

Verification: Are we solving the equations correctly?

- Represents an exercise in computational mathematics
- Given an equation, is the solution converging at known rates?

Validation: Are we solving the correct equations?

- Represents an exercise in understanding the physics associated with the real world use case

In this course, we will strongly focus on *verification*

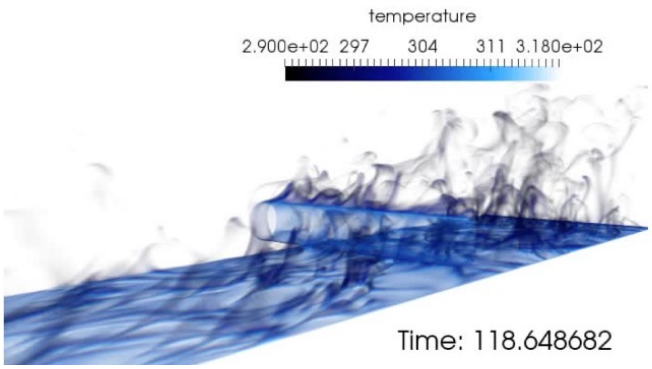
- Establishing the correctness of the numerical implementation is key
- Comparisons of the numerical results to reality is not the primary objective

Verification challenges?

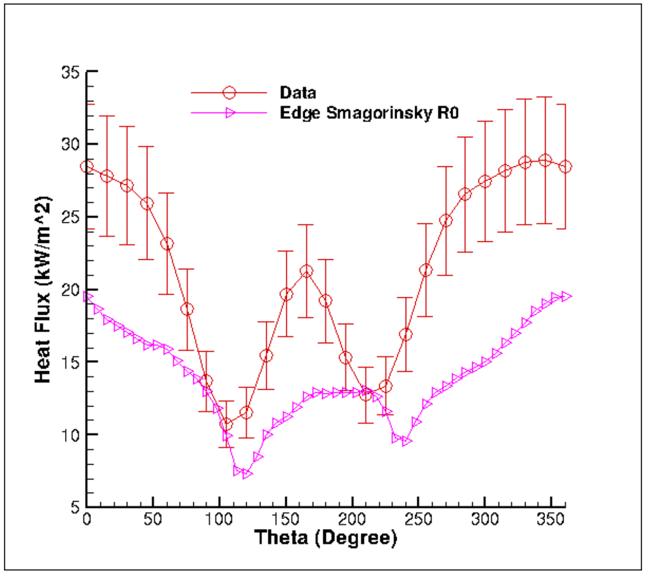
- Knowledge of the true solution, i.e., exact analytical solutions
- How many exact solutions exist for our class of physics? Not many!
- Hint: Method of Manufactured Solutions (MMS)

Challenge: Understanding Errors/Uncertainties….

- One mesh, one model, unknown code/numerical pedigree…
- We need to distinguish the types of errors/uncertainties:
  - Conceptual uncertainty, δ_{input}
  - Model-form error/uncertainty, δ_{model}
  - Discretization Error, $\delta_{numerical}$
  - Code Error, $\delta_{numerical}$



Heat flux to the cylinder
Volume-rendered temperature



Time-averaged heat flux to cylinder

- What credible scientific hypothesis can be tested in this context?

Review of the Method of Manufactured Solutions (MMS):

Providing confidence that the code implementation converges to the proper solution

- We understand that the number of analytical solutions to test our code implementation are very few in number
- How can we test the numerical accuracy of our implementation that, in general, solves very complex physics?
- Specifically, as we refine the mesh and time step, how does the error respond?

Consider a simple heat conduction PDE:

$$\rho C_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} = 0$$

With given [steady] manufactured solution:

$$T^{mms}(x,y,z) = \frac{k}{4\lambda}\left(cos(2\pi x) + cos(2\pi y) + cos(2\pi z)\right)$$

- New, analytically modified system that includes a new source term that we can implement in the code base:

$$\rho C_p \frac{\partial T^{mms}}{\partial t} - \frac{\partial}{\partial x_j} \lambda \frac{\partial T^{mms}}{\partial x_j} = S^{mms}$$

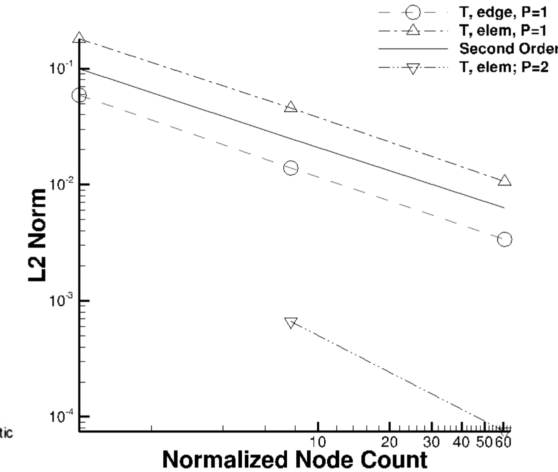
- The error is computed to be the difference between the analytical, or manufactured solution and our numerical simulation, T^h
- We can now refine the mesh and timestep, while computing the error to ensure that the rate of reduction is expected
- For example, if we believe our scheme is 2nd or 3rd order in space accuracy, one uniform refinement should reduce the error by 4x or 8x, respectively

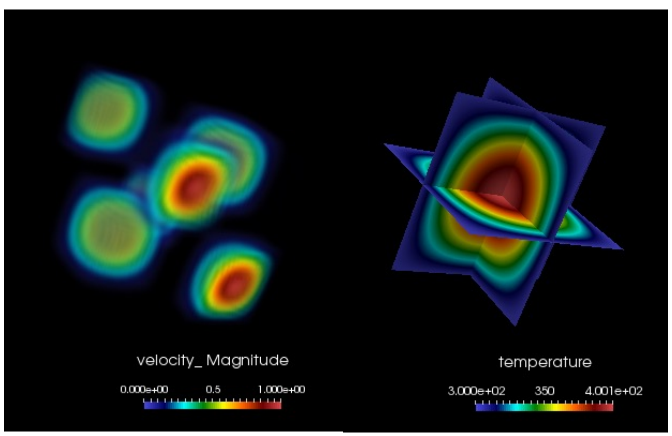
$$S^{mms}(x,y,z) = k\pi^2\left(cos(2\pi x) + cos(2\pi y) + cos(2\pi z)\right)$$

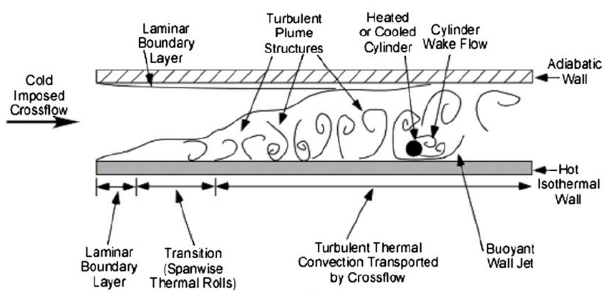
Spatial Code Verification for a low-Mach, Variable-Density Flow

	Import	Adequacy			
	Phen	Mod	Code	Val	Mats
Convective Processes					
Convective heat transfer	M	M	M	L	

- Density is a function of static enthalpy transport via the standard ideal gas, $\rho = f(P,M,R,T)$
- Temperature range maps to experiment (see below)
- Arbitrary buoyancy source term via rotated gravity vector
- Collective study now provides confidence in the interplay between numerical and modeling accuracy







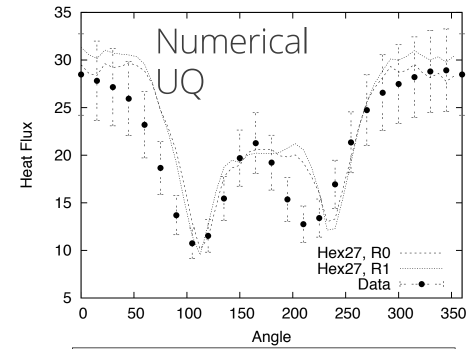
See, "Exploring model-form uncertainties in large-eddy simulations", Domino et al, 2016

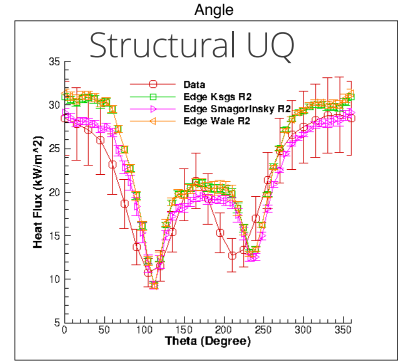
Velocity Mag   Temperature   Kearney experimental configuration

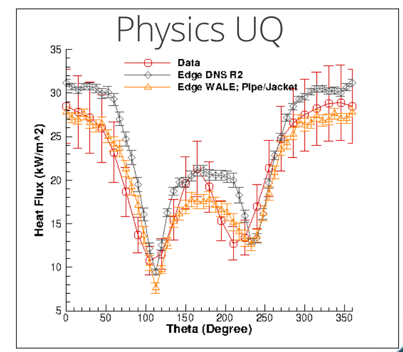
Review of a Strong V&V Process

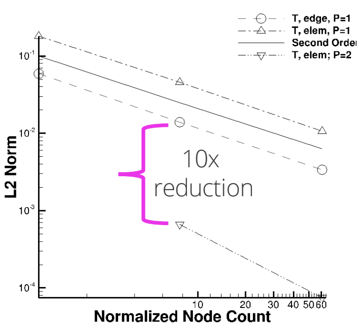
Establish a sound LES-based V&V process (with uncertainty quantification) that includes the following attributes:

- Phenomena Identification and Ranking (PIRT)
- Code and solution verification (numerical error, $\delta_{numerical}$)
- Validation including solution sensitivity to model inputs (δ_{input})
- Structural uncertainty (model form error, δ_{model})
- Physics assumptions (your conceptual model)

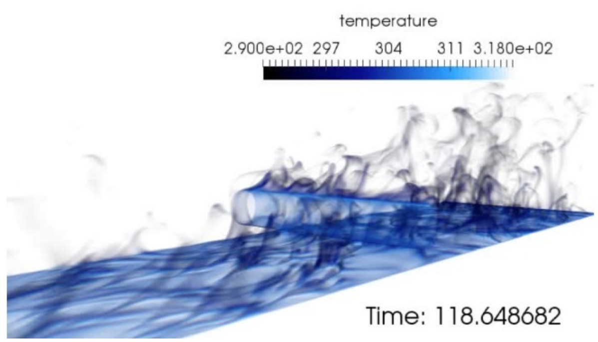








Non-isothermal MMS



Sources of error and uncertainty in simulation

$\delta_{numerical}$, δ_{input} , δ_{model}

"An assessment of atypical mesh topologies for low-Mach LES", Domino et al., *Comp & Fluids*, 2019

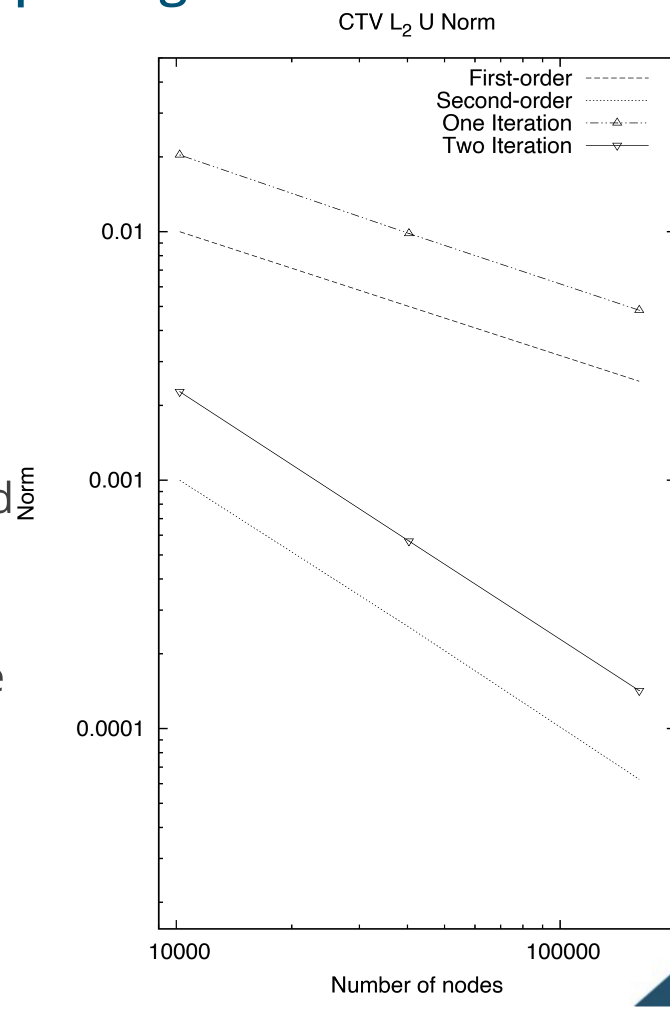
Code or Conceptual Error? Part 1: Time Splitting

Case Study: An Algorithm is thought to be second-order-in-time accurate with one nonlinear iteration: True or False?

- Issa, "Solution of the implicitly discretized fluid flow equations by operator splitting", JCP (1985).
  - Advent of the "Pressure-implicit with Splitting of Operators", or PISO
- PISO is a scheme that defines a series of predictors and correctors in the context of a fully implicit solve

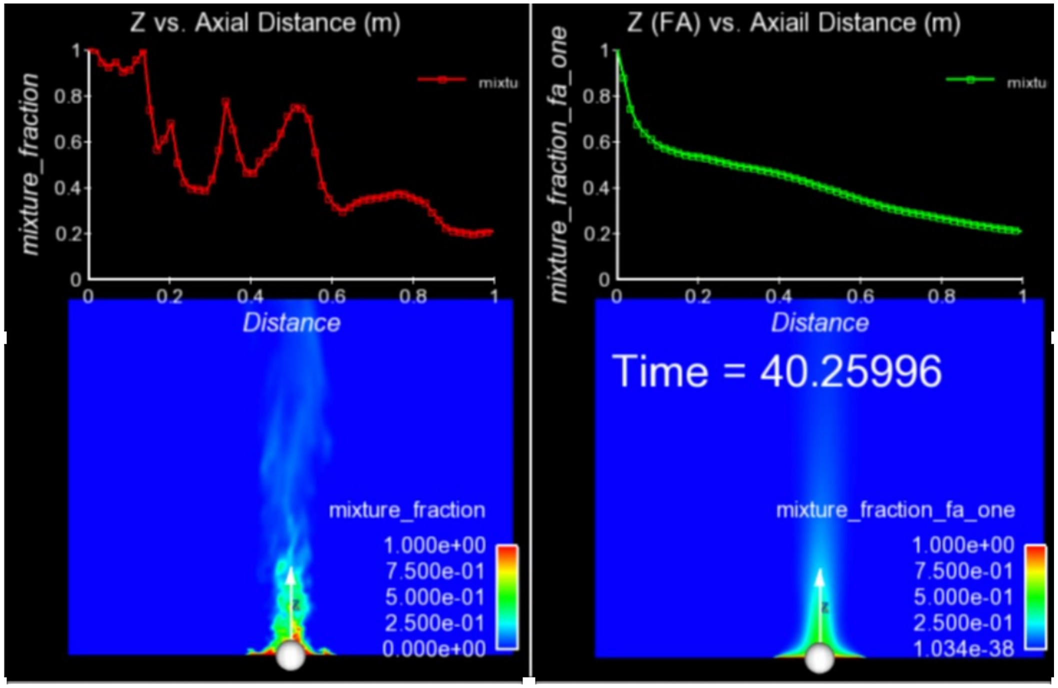
Conclusion?

- Sometimes we code a method correctly, however, have a conceptual error in our understanding of whether or not a scheme is design-order accurate when run in the suggested manner



Finally…. For Transient Flows, Averaging is Required

- The **bane** of turbulent validation: converged statistics require many flow-through times
- Statistical convergence of a given simulation may require many flow-through-times; additional source of uncertainty and/or requirement for quantification of solution convergence



Essentials of Code Verification: Review

<u>Taxonomy</u>: One *verifies* code and *validates* models

- Code verification establishes the numerical accuracy of the underlying discretization for the given partial differential equation set
- Code verification seeks to provide the temporal and spatial accuracy of the underlying discretization approach

For temporal discretization error,

- A two-state Backward Euler time integrator should be first-order in time, specifically the error should scale with Δt
- A three-state BDF2 time integrator should scale with Δt^2
- A multi-stake Runge-Kutta schemes can achieve higher-order accuracy

For spatial discretization error,

- A method is design-order if the observed order of accuracy is Δx^{P+1}, where P is the underlying basis polynomial order

Oberkampf and Trucano, Verification and validation in computational fluid dynamics, Progress in Aerospace Sciences, Volume 38, Issue 3, 2002, https://doi.org/10.1016/S0376-0421(02)00005-2.